Quantum Gates Based on Adiabatic Controlling Processes in a Silicon–Based Nuclear Spin Quantum Computer

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Kaneが提案した半導体核スピン量子コンピュータについてパラメータの断熱的変動による系の時間発展を詳細に解析し，その結果に基づき位相シフト演算，制御Z演算を実行するスキームを考察する．

1 Introduction

Various models for the experimental realization of quantum computation have been proposed [1]. Kane [2] proposed the quantum computation by nuclear spins in a semiconductor, where the nuclear spin of the dopant atom ^{31}P implanted into the silicon substrate is a single qubit and the quantum state is measured by detecting the charge of one electron around the donor (i.e., ^{31}P). Although the implantation of atoms with accuracy and the detection of the single electronic charge are very difficult even in the present state of technology, the Kane's proposal has the possibility of realizing quantum computation by the use of multi–qubits, applying the several existing micro fabrication techniques of semiconductors. Furthermore, the several important experimental techniques for the experimental realization of this proposal, for example, the single ion implantation method [3] and the single electron transistor [4], have been developed steadily.

In this paper, we discuss schemes for performing quantum gates in the Kane's model based on the adiabatic varying processes for the controllable parameters involving in it. So far, several authors have researched the construction of quantum gates proposed by Kane. Hill and Goan [5] showed the schemes of several single qubit operations, a controlled–Z gate and a controlled–NOT (CNOT) gate by instantaneously varying all parameters in the system, based on the perturbation theory for the controlling parameters. However, an instantaneous variation of parameters is only an idealized process in real experiments. Moreover, the potential errors could exist in their scheme since they analyze the system approximately. Fowler [6] *et al.* showed numerically the scheme of a CNOT gate based on the adiabatic controlling process for parameters and discussed the effect of decoherence for it. It is important to understand the reason why their scheme works successfully, comparing it with the more acceptable model than the original one. We analyze the Kane's model exactly when the rotating magnetic field is not applied, and show the scheme of a phase shift operation and a controlled–Z gate.

2 Quantum gates based on adiabatic controlling processes

The Kane's architecture, as is shown in Fig. 1, consists of the dopant atoms in a one dimensional array embedded in a silicon substrate, the gates (A–gates) located right above each dopant atom, and the other gates (J–gates) between the neighbouring dopant atoms.

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The Kane's model for two qubits is described by the Hamiltonian, $H^{(1,2)} = \sum_{i=1}^{2} H^i + J\boldsymbol{\sigma}^{1e} \cdot \boldsymbol{\sigma}^{2e} + \sum_{i=1}^{2} H^i_{ac}$, where $H^i = -g_n\mu_n B\sigma_z^{in} + \mu_B B\sigma_z^{ie} + A_i\boldsymbol{\sigma}^{ie} \cdot \boldsymbol{\sigma}^{in}$, $H^i_{ac} = B_{ac}\boldsymbol{m}^i \cdot (-g_n\mu_n\boldsymbol{\sigma}^{in} + \mu_B\boldsymbol{\sigma}^{ie})$, $\boldsymbol{m}^i = (\cos(\omega_{ac}t),\, \sin(\omega_{ac}t),\, 0)$, σ_k ($k = x,\, y,\, z$) is the Pauli Matrix, μ_B is the Bohr magnetic moment ($\mu_B B = 0.116\,\mathrm{meV}$), μ_n is the nuclear magnetic moment and g_n is the g–factor of $^{31}\mathrm{P}$ ($g_n\mu_n B = 0.071 \times 10^{-3}\,\mathrm{meV}$). The superscript e (n) in the Pauli matrix indicates the electronic (nuclear) spin. The hyperfine interaction (HY) between the i–th nuclear spin and the i–th electronic spin is $A_i\boldsymbol{\sigma}^{ie} \cdot \boldsymbol{\sigma}^{in}$ and is locally changed by controlling the voltage of the i–th A–gate. The value of the HY is $0.121 \times 10^{-3}\,\mathrm{meV}$ ($\equiv A_0$) when the voltage of the A–gate is vanishing, and the magnitude of A_i weakens as the voltage of the i–th A–gate decreases [2]. The electronic exchange interaction (EE) between the 1st and the 2nd electronic spins is $J\boldsymbol{\sigma}^{1e} \cdot \boldsymbol{\sigma}^{2e}$ and is locally changed by controlling the voltage of J–gate. We assume that it will be possible to change the magnitude of the EE from $J = 0\,\mathrm{meV}$ to $J \simeq \mu_B B$ [2, 5]. The third term in $H^{(1,2)}$ is the rotating magnetic field, and plays important role in spin flip operations [2]. Hereafter, we calculate the temporal behavior in the system when the rotating magnetic field is not applied.

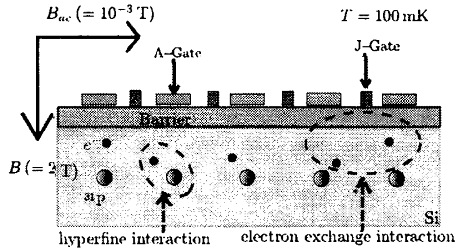

FIG. 1: The sketch of the Kane's architecture. The dopant atoms are implanted at 20 nm intervals. The static magnetic field is uniformly applied in the direction of z–axis and the magnitude of it is 2 T. Furthermore, the rotating magnetic field is applied in a direction perpendicular to z axis and the magnitude of it is about 10^{-3} T. Temperature of the device is 100 mK.

Before calculating the time evolution of the system by adiabatically varying parameters, we have to choose the suitable states to represent a qubit. Note that, in Ref. [5], the electrons are assumed to be always polarized in the downward direction. However, this choice is not so good for the A–gate operation. The logical states ($|0\rangle_{L,i}$ and $|1\rangle_{L,i}$) of the i–th qubit should consist of the eigenstates for H^i: $|0\rangle_{L,i} \equiv |u_1^i\rangle$ and $|1\rangle_{L,i} \equiv |u_0^i\rangle$, where $|u_0^i\rangle$ and $|u_1^i\rangle$ are the ground state and the first excited state of H^i, respectively. These states are no longer the eigenstates for σ_z^{in} or σ_z^{ie}, because the value of the HY is non–zero. When we calculate the energy difference Δ_{01}^i between $|u_1^i\rangle$ and $|u_0^i\rangle$, we find that $\Delta_{01}^i \simeq 2A_i + 2g_n\mu_n B$; it is characterised by the magnitude of the HY. Therefore, the phase difference between $|u_1^i\rangle$ and $|u_0^i\rangle$ is controlled by varying the value of A_i. Next, let us explain the relationship between the above logical states and the eigenstates of $H^{(1,2)}$. We introduce the total spin operator $S = (\sigma_z^{1n} + \sigma_z^{1e} + \sigma_z^{2n} + \sigma_z^{2e})/2$ and the parity operator P which permutates the index of qubit (i.e., i) between the identical particles. We find that $[S,\, H^{(1,2)}] = [P,\, H^{(1,2)}] = 0$ and $H^{(1,2)} = \oplus_{s,p}H(s,p)$, where $s(= -2, -1, 0, 1, 2)$ and $p(= +-)$ are the quantum numbers for S and P, respectively, if the rotating magnetic field is not applied and $A_1 = A_2$. Non–zero parts of each $H(s,p)$ are 4×4 matrices at most. Therefore, the Hamiltonian $H^{(1,2)}$ is diagonarized analytically. Introducing $|v_1\rangle \equiv |0\rangle_{L,1}|0\rangle_{L,2}$, $|v_\pm\rangle \equiv (|0\rangle_{L,1}|1\rangle_{L,2} \pm |1\rangle_{L,1}|0\rangle_{L,2})/\sqrt{2}$, and $|v_4\rangle \equiv |1\rangle_{L,1}|1\rangle_{L,2}$, we find that $|v_1\rangle$, $|v_+\rangle$, $|v_-\rangle$, and $|v_4\rangle$ are the eigenstates of $H(0,+)$, $H(-1,+)$, $H(-1,-)$, and $H(-2,+)$, respectively, if the value of J is vanishing.

We achieve the phase shift operation for the i–th qubit, keeping $J(t) = 0$ and $A_j(t) = A_0$ ($j \neq i$), and varying $A_i(t)$ adiabatically. Introducing two parameters a ($0 < a < 8$) and $T_{op}(> 0)$, we assume the time dependence of $A_i(t)$ as follows: $A_i(t) = A_0(1 - a\tau^2)$ for $0 < \tau < 1/4$, $A_i(t) = A_0(1 - a/8 + a(\tau - 1/2)^2)$ for $1/4 < \tau < 1/2$, and $A_i(t) = A_0(1 - a(\tau - 1/2)^2)$ for $3/4 < \tau < 1$, where $\tau = t/T_{op}$. The parameter T_{op} is just the operation time for the phase shift operation. The parameter a is a dimensionless number. The initial state for the i–th qubit is spanned by $|u_0\rangle$

and $|u_1\rangle$. Therefore, the time evolution operator $U^i(T_{op})$ for the i–th qubit, due to the adiabatic theorem, is written by $U^i(T_{op}) = T\left[\exp(-i\hbar^{-1}\int_0^{T_{op}} H^i(t)\,dt)\right] \approx e^{-i\delta_0^i}|u_0^i\rangle\langle u_0^i| + e^{-i\delta_1^i}|u_1^i\rangle\langle u_1^i|$, where $\delta_0^i = T_{op}\{\int_0^1(-A_i(s) - \sqrt{(g_n\mu_n B + \mu_B B)^2 + 4A_i(s)^2})\,ds\}/\hbar$ and $\delta_1^i = T_{op}\big(g_n\mu_n B - \mu_B B + \int_0^1 A_i(s)\,ds\big)/\hbar$. Generally, the terms related to $|u_1^i\rangle\langle u_2^i|$ appears in $U^i(T_{op})$ due to the structure of H^i, where $|u_2^i\rangle$ is the 2nd excited state of H^i. Let us write the adiabatic eigenstate of $H^{(i)}(t)$ for each instant of time as $|u_1^i(t)\rangle$ (i.e., $H^i(t)|u_1^i(t)\rangle = E_1^i(t)|u_1^i(t)\rangle$), and so on. The energy difference between $|u_1^i(t)\rangle$ and $|u_2^i(t)\rangle$ is characterized by the value of $\mu_B B$. Therefore, the adiabatic approximation for the above $A_i(t)$ is valid. On the other hand, because the maximum value of $|A_i'(t)|$ is characterized by a quantity which is smaller than the value of $\mu_B B$. We obtain the two conditions of the parameters a and T_{op}: (i) $\delta_0^i - \delta_1^i = 2n\pi + \theta$ (i.e., the condition to obtain the phase difference θ between $|0\rangle_{L,i}$ and $|1\rangle_{L,i}$ for the i–th qubit) and (ii) $\delta_0^j - \delta_1^j = 2m\pi$ (i.e., the condition to obtain no phase difference between $|0\rangle_{L,j}$ and $|1\rangle_{L,j}$ for the other qubits), where m and n are some integers.

Next, we construct the controlled–Z gate, keeping $A_1 = A_2 = A_0$, varying $J(t)$ adiabatically. Introducing four parameters $J_c(>0)$, $T_a(>0)$, $T_h(>0)$, and τ_c $(0 < \tau_c < 1/2)$, we assume the time dependence of $J(t)$ as follows: $J(t) = J_c\xi\tau^2$ for $0 < \tau < \tau_c$, $J(t) = J_c(1 - \eta(\tau - 1/2)^2)$ for $\tau_c < \tau < 1/2$, $J(t) = J_c$ for $1/2 < \tau < \tau_h + 1/2$, $J(t) = J_c(1 - \eta(\tau - \tau_h - 1/2)^2)$ for $\tau_h + 1/2 < \tau < \tau_c + \tau_h + 1/2$, and $J(t) = J_c\xi(\tau - 1 - \tau_h)^2$ for $\tau_c + \tau_h + 1/2 < \tau < \tau_h + 1$, where $\xi = 2/\tau_c$, $\eta = 4/(1 - 2\tau_c)$, $\tau = t/T_a$, and $\tau_h = T_h/T_a$. The operation time T_{op} for the controlled–Z gate is given by $T_{op} = T_a + T_h$. The parameter J_c is the maximum value of $J(t)$. The parameter τ_c is a dimensionless number. The initial state for the two qubis is spanned by $|v_1\rangle$, $|v_\pm\rangle$, and $|v_4\rangle$. Therefore, the time evolution operator for the two qubits, due to the adiabatic theorem, is described by $U^{(1,2)}(T_{op}) = T\left[\exp(-i\hbar^{-1}\int_0^{T_{op}} H^{(1,2)}(t)\,dt)\right] \approx \sum_k e^{-i(\alpha_k+\beta_k)}|v_k\rangle\langle v_k| = \left(\sum_k e^{-i\alpha_k}|v_k\rangle\langle v_k|\right)\left(\sum_j e^{-i\beta_j}|v_j\rangle\langle v_j|\right)$. We obtain the analytical expressions for α_k and β_j $(k, j = 1, +, -, 4)$, but we don't write these explicitly in this paper because they are rather complicated expressions composed of the eigenvalues of $H^{(1,2)}$. The phase α_k and β_k are related to the process under which the value of $J(t)$ changes and the value of $J(t)$ is constant, respectively. The adiabatic approximation is valid for $J_c < 0.5\mu_B B$ in our assumption for $J(t)$, because there are the adiabatic eigenstates of $H^{(1,2)}$ between which the energy difference is characterized by the value of A_0 as $J(t) \to 0.5\mu_B B$. Let us write $U_{adc} \equiv \sum_k e^{-i\alpha_k}|v_k\rangle\langle v_k|$ and $U_{stat} = \sum_k e^{-i\beta_k}|v_k\rangle\langle v_k|$. We obtain the conditions that U_{adc} is equal to the single qubit operation $(\sigma_z^1 \otimes \mathbb{1}^2)(\mathbb{1}^1 \otimes \sigma_z^2)$ $(\sigma_z^i = |0\rangle_{L,i}\langle 0| - |1\rangle_{L,i}\langle 1|$ and $\mathbb{1}^i = |0\rangle_{L,i}\langle 0| + |1\rangle_{L,i}\langle 1|)$ as follows: $\alpha_1 - \alpha_\pm = \pi + 2m_\pm\pi$ and $\alpha_1 - \alpha_4 = 2m_4\pi$, where $m_\pm$ and m_4 are some integers. In general, a controlled-Z gate $U_{cz}(\theta)$ of the angle θ is $U_{cz}(\theta) = e^{-i\frac{\theta}{2}\sigma_z^1\otimes\sigma_z^2}(\mathbb{1}^1 \otimes e^{i\frac{\theta}{2}\sigma_z^2})$. A controlled–Z gate is $U_{cz}(\theta = \pi/2)$. The operation $e^{-i\frac{\pi}{4}\sigma_z^1\otimes\sigma_z^2}$ between the two qubits consists of U_{stat} and the phase shift operations and several spin flip operations. According to Ref. [5], we obtain the final condition to determine the parameters as follows: $2(\beta_+ - \beta_-) = \pi$. Therefore, the controlled–Z gate in our scheme consists of the gate by instantaneously varying the parameters in Ref. [5] and the correction term U_{adc}.

3 Numerical results

We show the results for the phase shift operation. We solve the equations of a and T_{op} for given θ numerically. The integers m and n are free parameters. We show the results for $m = -5$ and $n = -6$ in Table I, where the value of A_{min} is a minimum value of $A_i(t)$ and $A_{min} = A_0(1 - a/8)$. The operation time T_{op} is independent of the value of θ, and 0.05 μs for $m = -5$, which is almost equal to the result in Ref. [5]. We find that the phase shift operations are performed by varying the HY up to $A_0/2$ at most.

Next, we calculate the values of J_c and τ_c such that the operator U_{adc} is equivalent to $(\sigma_z^1 \otimes$

θ	$\pi/4$	$\pi/2$	$3\pi/4$	π
a	4.78	5.31	5.84	6.37
A_{min}/A_0	0.402	0.336	0.270	0.203

TABLE I: The values of a and A_{min} for $\theta = \pi/4, \pi/2$, $3\pi/4$, and π. The value of the free parameters m and n for any θ are -5 and -6, respectively.

$\mathbb{1}^2)(\mathbb{1}^1 \otimes \sigma_z^2)$, by numerically solving equations $(\alpha_1 - \alpha_4)/(\alpha_1 - \alpha_\pm) = 2m_4/(1 + 2m_\pm)$. We find that several solutions exist; for example, $J_c/\mu_B B = 0.1988$ (i.e., $J_c \simeq 0.023\,\mathrm{meV}$) and $\tau_c = 0.1925$ for $m_4 = 1$ and $m_\pm = 0$. The maximum value of $J(t)$ is 0.0423 meV in Ref. [5] and 0.056 meV in Ref. [6]. Our results are rather smaller than those values.

4 Discussion

In this paper, the schemes of the phase shit operation and the controlled–Z gate in the Kane's model have been researched, based on the adiabatic controlling processes of the parameters. The phase shift operation for the i–th qubit is performed by varying $A_i(t)$ adiabatically. Its operation time is estimated at about $10^{-2}\,\mu$s. The controlled–Z gate consists of two time evolution operators U_{stat} and U_{adc}: The element of controlled operations between two qubits involved in U_{stat}. On the other hand, U_{adc} is equivalent to the single qubit operation $(\sigma_z^1 \otimes \mathbb{1}^2)(\mathbb{1}^1 \otimes \sigma_z^2)$, by adjusting the time dependence of the parameter. Actually, we have to use many spin flip operations in the scheme of the controlled–Z gate. However, our recent calculation suggests that there are potentially errors in the spin flip operations of the Kane's original proposal. And, it is important to research the temporal behavior of the system for $J(t) > \mu_B B/2$, because it is necessary to vary the value of it from 0 to $\mu_B B$ in the measurement scheme of the Kane's model. In future, we would like to research the origin of such errors in detail.

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